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Supporting Information

Prediction Models of P-Glycoprotein Substrates Using Simple 2D and 3D Descriptors Bya Recursive Partitioning Approach

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Prediction Results of 2D and 3D RP classification models

	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	CNC(=O)O₩N=C₩C(C)(C)SC	Non_sub	Non_sub	Non_sub	carbamate insecticide
b	CNC(=O)O₩N=C₩C(C)(C)S(=O)(=O)C	Non_sub	Non_sub	Non_sub	pesticide
ne	NC12CC3CC(CC(C3)C1)C2	Non_sub	Non_sub	Non_sub	antiparkinsonian drug
b	CNC(=O)Oc1ccc(N(C)C)c(C)c1	Non_sub	Non_sub	Non_sub	pesticide
e	CN1N(C(=O)C=C1C)c2ccccc2	Non_sub	Non_sub	Non_sub	analygesic, antipyretic drug
	CC(C)NCC(O)COc1ccc(CC(=O)N)cc1	Non_sub	Non_sub	Non_sub	selective beta1 receptor antagonist
	CCNc1nc(Cl)nc(NC(C)C)n1	Non_sub	Non_sub	Non_sub	herbicide
	C[C@@H]1CN(C[C@H](C)O1)c2nc(N(CC O)CC(C)(C)O)c3nc(c4ccccc4)c(nc3n2)N5 C[C@@H](C)O[C@@H](C)C5	Non_sub	Sub	Sub	multidrug resistance-reversing agent
	OC(CCN1CCCCC1)(C2CC3CC2C=C3)c4cc ccc4	Non_sub	Sub	Non_sub	antiparkinsonian agen (anticholinergic type
	CNC(=O)Oc1cccc2ccccc12	Non_sub	Non_sub	Non_sub	insecticide
in	OC(=O)C1(CCC1)C(=O)O	Non_sub	Non_sub	Non_sub	anti-cancer drug
ne	ClCCNC(=O)N(CCCl)N=O	Non_sub	Non_sub	Non_sub	mustard gas-related β-chloro-n compound used as an alkylating chemotherapy
	C[C@H](CCC(=O)NCCC[N+](C)(C)CCCS(=O)(=O)[O-])[C@H]1CC[C@H]2[C@@H]3[C@H](O) C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C	Non_sub	Non_sub	Sub	detergent
ucil	OC(=O)CCCc1ccc(cc1)N(CCCl)CCCl	Non_sub	Non_sub	Non_sub	anti-leukemia drug, treating chronic lyı leukemia
iramine	CN(C)CCC(c1ccc(Cl)cc1)c2ccccn2	Non_sub	Non_sub	Non_sub	antihistamine drug

	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	Clc1cccc(Cl)c1NC2=NCCN2	Non_sub	Non_sub	Non_sub	alpha2 adrenergic agonist, treating hig pressure, ADHD, anxiety/panic disorder
ne	C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@H]2CC[C@@]4(C)[C@H]3CC[C@]4(O)C(=O)CO	Non_sub	Sub	Sub	selective androgen antagonist
sphamide	ClCCN(CCCl)P1(=O)NCCCO1	Non_sub	Non_sub	Non_sub	anticancer drug
e	NC1=NC(=O)N(C=C1)[C@@H]2O[C@H](CO)[C@@H](O)[C@@H]2O	Non_sub	Non_sub	Non_sub	anti-leukemia drug, treating acute myeloid
ticosterone	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2C(=O)CO	Non_sub	Sub	Sub	steroid hormone
lophyllotoxin	COc1cc(cc(OC)c1OC)[C@H]2[C@@H]3[C@H](COC3=O)Cc4cc5OCOc5cc24	Non_sub	Non_sub	Non_sub	treating passive cutaneous anaphylaxis rea
	CCOP(=S)(OCC)SC(CCl)N1C(=O)c2ccccc2C1=O	Non_sub	Non_sub	Non_sub	pesticide
	ClC1=C(Cl)[C@]2(Cl)C3[C@H]4C[C@H](C5OC45)C3[C@]1(Cl)C2(Cl)Cl	Non_sub	Non_sub	Non_sub	insecticide
ne	CN(C)CCOC(C)(c1ccccc1)c2ccccn2	Non_sub	Non_sub	Non_sub	antihistamine drug
ne	CNC[C@H](O)c1ccc(O)c(O)c1	Non_sub	Non_sub	Non_sub	hormone, neurotransmitter
hyllotoxin	COc1cc(cc(OC)c1OC)[C@H]2[C@@H]3[C@H](COC3=O)[C@H](O)c4cc5OCOc5cc24	Non_sub	Sub	Non_sub	natural alkaloid, anti-leukemia
butyl	CCCCOC(=O)C(C)Oc1ccc(Oc2ccc(cn2)C(F)(F)F)cc1	Non_sub	Non_sub	Non_sub	pesiticide
il	CCOC(=O)c1ncn2c1CN(C)C(=O)c3cc(F)ccc23	Non_sub	Non_sub	Non_sub	benxodiazepine antagonist, antidote treatment of benzodiazepine overdose
cil	FC1=CNC(=O)NC1=O	Non_sub	Non_sub	Non_sub	anticancer drug, inhibitor of thymidylate sy
nz	NC(=N₩N=C₩c1c(Cl)cccc1Cl)N	Non_sub	Non_sub	Non_sub	antihypertensive drug

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
Guanfacine	NC(=NC(=O)Cc1c(Cl)cccc1Cl)N	Non_sub	Non_sub	Non_sub	lagonist of the alpha-2A subtype of norepinephrine receptors, lowering systolic and diastolic blood pressure by activating the central nerve systems
Imipramine	CN(C)CCCN1c2ccccc2CCc3ccccc13	Non_sub	Non_sub	Non_sub	antidepressant
Indomethacin	COc1ccc2c(c1)c(CC(=O)O)c(C)n2C(=O)c3ccc(Cl)cc3	Non_sub	Non_sub	Non_sub	non-steroidal anti-inflammatory drug, reducing fever, pain, stiffness
Itraconazole	CCC(C)N1N=CN(C1=O)c2ccc(cc2)N3CCN(CC3)c4ccc(OC[C@H]5CO[C@@](Cn6cncn6)(O5)c7ccc(Cl)cc7Cl)cc4	Non_sub	Non_sub	Non_sub	antifungal agnet. Preventing the fungi from producing the membranes that surround the fungal cells
Ketamine	CNC1(CCCCC1=O)c2ccccc2Cl	Non_sub	Non_sub	Non_sub	veterinary midicine
Ketoconazole	CC(=O)N1CCN(CC1)c2ccc(OC[C@H]3CO[C@@](Cn4ccnc4)(O3)c5ccc(Cl)cc5Cl)cc2	Non_sub	Non_sub	Non_sub	synthetic antifungal drug, treating fungal skin infection
Leptophos	COP(=S)(Oc1cc(Cl)c(Br)cc1Cl)c2ccccc2	Non_sub	Non_sub	Non_sub	organophosphate pesticide
Lidocaine	CCN(CC)CC(=O)Nc1c(C)cccc1C	Non_sub	Non_sub	Non_sub	anesthetic, antiarrhythmic drug
Lindane	ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	Non_sub	Non_sub	Non_sub	agricultural insecticide, anti-lice, anti-scabies drug
Mannitol	OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	Non_sub	Non_sub	Non_sub	osmotic diuretic drug
Mebendazole	COC(=O)Nc1nc2ccc(cc2[nH]1)C(=O)c3ccccc3	Non_sub	Non_sub	Sub	antiworm, anti-parasite drug
Mephentermine	CNC(C)(C)Cc1ccccc1	Non_sub	Non_sub	Non_sub	cadiac stimulant
Meprobamate	CCCC(C)(COC(=O)N)COC(=O)N	Non_sub	Non_sub	Non_sub	anxiolytic drug, treating anxiety disorders
Methoxychlor	COc1ccc(cc1)C(c2ccc(OC)cc2)C(Cl)(Cl)Cl	Non_sub	Non_sub	Non_sub	pesticide
Metoprolol	COCCc1ccc(OCC(O)CNC(C)C)cc1	Non_sub	Non_sub	Non_sub	selective beta1 receptor blocker, treating diseases of cadiovascular system
Mevinphos	COC(=O)₩C=C(/C)₩OP(=O)(OC)OC	Non_sub	Non_sub	Non_sub	organophosphate insecticide
Mexiletine	CC(N)COc1c(C)cccc1C	Non_sub	Non_sub	Non_sub	antiarrhythmic drug

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
Midazolam	Cc1ncc2CN=C(c3ccccc3F)c4cc(Cl)ccc4n12	Non_sub	Non_sub	Non_sub	treating acute seizures, moderate to severe insomnia
Mirex	ClC1(Cl)C2(Cl)C3(Cl)C4(Cl)C(Cl)(Cl)C5(Cl)C(Cl)(C1(Cl)C35Cl)C24Cl	Non_sub	Non_sub	Non_sub	insecticide
Naloxone	Oc1ccc2C[C@H]3N(CC=C)CC[C@@]45[C@@H](Oc1c24)C(=O)CC[C@@]35O	Non_sub	Sub	Sub	opioid antagonist, blocking the actions of opioid medicine
Naltrexone	Oc1ccc2C[C@H]3N(CC4CC4)CC[C@@]56[C@@H](Oc1c25)C(=O)CC[C@@]36O	Non_sub	Sub	Sub	-
Nigericin	CO[C@@H]1C[C@@H](C[C@H]2CC[C@H](C)[C@@H](O2)[C@@H](C)C(=O)O)O[C@]3(O[C@@](C)(C[C@H]3C)[C@H]4CC[C@](C)(O4)[C@@H]5O[C@H](C[C@@H]5C)[C@H]6O[C@@](O)(CO)[C@H](C)C[C@@H]6C)[C@@H]1C	Non_sub	Sub	Sub	antibiotics
Nitrazepam	[O-][N+](=O)c1ccc2NC(=O)CN=C(c3ccccc3)c2c1	Non_sub	Non_sub	Non_sub	-
Nitrendipine	CCOC(=O)C1=C(C)NC(=C(C1c2cccc(c2)[N+](=O)[O-])C(=O)OC)C	Non_sub	Sub	Sub	-
Nordazepam	Clc1ccc2NC(=O)CN=C(c3ccccc3)c2c1	Non_sub	Non_sub	Non_sub	anti-anxiety agent, treating anticonvulsant, anxiolytic, muscle relaxant sedative properties
NSC268251	CC(C)CCCCCCCCCCCC(=O)NCC(=O)NC1C(C)OC(Nc2ncnc3nc[nH]c23)C(O)C1O	Non_sub	Non_sub	Sub	-
NSC309132	OCC1OC(C(O)C1O)N2C=CC=NC2=O	Non_sub	Non_sub	Non_sub	-
NSC314622	COc1cc2C(=O)N(C)C3=C(C(=O)c4cc5OCOc5cc34)c2cc1OC	Non_sub	Non_sub	Non_sub	-
NSC364080	CC1C(N(C)C(C(C)C1=O)c2ccccc2)c3ccccc3	Non_sub	Non_sub	Non_sub	-

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
NSC49899	CCOC(=O)C1C(N(C)C(C(C(=O)OCC)C1=O)c2ccccc2)c3ccccc3	Non_sub	Sub	Sub	-
NSC606532	COc1cc(c(cc1N)[N+](=O)[O-])[N+](=O)[O-]	Non_sub	Non_sub	Non_sub	-
NSC615985	CC(C)OC(=O)c1cc(NC(=O)C2=C(C)OCCS2)ccc1Cl	Non_sub	Sub	Sub	-
NSC617286	O=C(OCc1ccccc1)OOC(=O)OCc2ccccc2	Non_sub	Non_sub	Non_sub	-
NSC623083	COc1ccccc1NS(=O)(=O)c2cc(ccc2OCCOc3ccc(cc3S(=O)(=O)Nc4ccccc4OC)C(C)(C)C)C(C)(C)C	Non_sub	Non_sub	Sub	-
NSC630148	CC(C)C(=O)NC(C)C(=O)N(Cc1ccc2ccccc2c1)N=O	Non_sub	Sub	Sub	-
NSC630357	CC(C(=NNC(=O)c1c(O)ccc2ccccc12)CCC(=O)Nc3cc(C)ccc3C)C(=O)c4ccc(O)cc4	Non_sub	Sub	Non_sub	-
NSC630721	Cc1cc(C)nc(NS(=O)(=O)c2ccc(NC(=O)COC(=O)c3cccc4C(=O)c5ccccc5Nc34)cc2)n1	Non_sub	Non_sub	Sub	-
NSC633528	CN(C)CCCCN1CCc2c(C1=O)n(C)c3ccccc23	Non_sub	Non_sub	Non_sub	-
NSC639677	Clc1ccccc1CN2N=C3C=CC=CC3=CC2=O	Non_sub	Non_sub	Non_sub	-
NSC648403	CS(=O)(=O)c1c(N)c2nc(Cl)cn2c3nc4ccccc4nc13	Non_sub	Sub	Sub	-
NSC653278	COc1ccc(cc1)C(=O)C(C(=O)c2ccc(OC)cc2)c3c(C(=O)c4ccc(OC)cc4)c5ccccc5n3C(=O)c6ccc(OC)cc6	Non_sub	Non_sub	Non_sub	-
NSC664565	CC1C=C(C)c2ccccc2N(CC3=NCCN3)C1C	Non_sub	Non_sub	Sub	-
NSC666331	CC1=CC(=C(C#N)C(=S)N1C2OC(CO)C(O)C(O)C2O)c3occc3	Non_sub	Non_sub	Non_sub	-

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
NSC667532	OC[C@@H]1O[C@@H]([C@@H](O)[C@@H](O)C1O)N2C3=C(CCCC3)C(=C(C#N)C2=S)c4occc4	Non_sub	Non_sub	Non_sub	-
NSC667533	CCOC(=O)C1=C(C)N(C2OC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C2OC(=O)C)C(=S)C(=C1c3ccc(Cl)cc3)C#N	Non_sub	Non_sub	Non_sub	-
NSC667551	CC(=O)C1=C(C)N(C2OC(CO)C(O)C(O)C2O)C(=S)C(=C1c3occc3)C#N	Non_sub	Non_sub	Non_sub	-
NSC667558	COc1ccc(cc1)C2=C(C#N)C(=S)N([C@@H]3O[C@H](COC(=O)C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@H]3OC(=O)C)C(=C2C(=O)C)c4ccccc4	Non_sub	Non_sub	Non_sub	-
NSC667560	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N2C(=C(C(=O)C)C(=C(C#N)C2=S)c3occc3)C	Non_sub	Non_sub	Non_sub	-
NSC668354	COc1ccc(CC2=C(C3C(=O)N(N=C3c4ccccc4)c5ccccc5)C(=O)NN=C2c6ccc(C)cc6)cc1	Non_sub	Sub	Sub	-
NSC671400	S=C1N(₩C(=N/c2cccc[n+]2Cc3ccccc3)₩N(/C/1=N/c4ccccc4)c5ccccc5)c6ccccc6	Non_sub	Non_sub	Non_sub	-
NSC674508	Cc1cc(C)nc(NS(=O)(=O)c2ccc(Nc3c4ccccc4nc5c(cccc35)C(=O)NNCCO)cc2)n1	Non_sub	Non_sub	Sub	-
NSC674570	COc1ccccc1C2SCC(=O)N2c3ccc(cc3)c4ccc(cc4)N5C(=O)c6ccccc6N=C5c7ccccc7	Non_sub	Non_sub	Non_sub	-
NSC676593	COc1ccc(cc1)C2=C(C#N)C(=S)N(C3OC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C3OC(=O)C)C4=C2C(=O)CC(C)(C)C4	Non_sub	Non_sub	Non_sub	-
NSC676602	CC1=C(C#N)C(=S)N(C2OC(CO)C(O)C(O)C2O)C(=C1)C	Non_sub	Non_sub	Non_sub	-

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
NSC676610	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N2C3=C(CCCC3)C=C(C#N)C2=S	Non_sub	Non_sub	Non_sub	-
NSC676615	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N2C3=C(CCCCCC3)C=C(C#N)C2=O	Non_sub	Non_sub	Non_sub	-
NSC676616	OCC1OC(C(O)C(O)C1O)N2C3=C(CCCCCC3)C=C(C#N)C2=S	Non_sub	Non_sub	Non_sub	-
NSC676617	OCC1OC(C(O)C(O)C1O)N2C3=C(CCCC3)C=C(C#N)C2=S	Non_sub	Non_sub	Non_sub	-
NSC676618	OCC1OC(C(O)C(O)C1O)N2C3=C(CCC3)C=C(C#N)C2=S	Non_sub	Non_sub	Non_sub	-
NSC678047	OCC1OC(C(O)C(O)C1O)N2C(=S)C(=C3C(=C2c4cccs4)CCc5ccccc35)C#N	Non_sub	Non_sub	Non_sub	-
NSC686028	CSC1=NC(=O)C(=C(N1)c2ccc(C)cc2)C#N	Non_sub	Non_sub	Sub	-
Oxprenolol	CC(C)NCC(O)COc1ccccc1OCC=C	Non_sub	Non_sub	Non_sub	treatment of angina pectoris, abnormal heart rhythms and high blood pressure
Paraquat	C[n+]1ccc(cc1)c2cc[n+](C)cc2	Non_sub	Non_sub	Non_sub	herbicides
Pheniramine	CN(C)CCC(c1ccccc1)c2ccccn2	Non_sub	Non_sub	Non_sub	antihistamine with anticholinergic properties used to treat allergic conditions such as hay fever or urticaria
Phosmet	COP(=S)(OC)SCN1C(=O)c2ccccc2C1=O	Non_sub	Non_sub	Non_sub	phthalimide-derevied, non-systemic, organophosphate insecticide used on plants and animals
Practolol	CC(C)NCC(O)COc1ccc(NC(=O)C)cc1	Non_sub	Non_sub	Non_sub	emergent treatment of cardiac arrhythmias
progesterone	CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12	Non_sub	Non_sub	Non_sub	hormone

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	C				
Propranolol	CC(C)NCC(O)COc1cccc2ccccc12	Non_sub	Non_sub	Sub	sympatholytic non-selective beta blocker, treating hypertension, anxiety and panic
PSC833	C₩C=C₩C[C@@H](C)C(=O)[C@@H]1N(C)C(=O)[C@H](C(C)C)N(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@@H](C)NC(=O)[C@H](C)NC(=O)[C@H](CC(C)C)N(C)C(=O)[C@@H](NC(=O)[C@H](CC(C)C)N(C)C(=O)CN(C)C(=O)[C@@H](NC1=O)C(C)C)C(C)C	Non_sub	Non_sub	Non_sub	-
Pyridostigmine	CN(C)C(=O)Oc1ccc[n+](C)c1	Non_sub	Non_sub	Non_sub	parasympathomimetic and a reversible cholinesterase inhibitor
Ranitidine	CN₩C(=C/[N+](=O)[O-])₩NCCSCc1oc(CN(C)C)cc1	Non_sub	Sub	Non_sub	histamine H2-receptor antagonist, inhibiting stomach acid production
reserpic_acid	CO[C@H]1[C@H](O)C[C@@H]2CN3CCc4c([nH]c5cc(OC)ccc45)[C@H]3C[C@@H]2[C@@H]1C(=O)O	Non_sub	Sub	Sub	a derivative of antihypertensive drug resperpine
Scopolamine	CN1[C@H]2CC(C[C@H]1[C@H]3O[C@@H]23)OC(=O)C(CO)c4ccccc4	Non_sub	Non_sub	Non_sub	tropane alkaloid drug with muscarinic antagonist effect
Selegiline	C[C@H](Cc1ccccc1)N(C)CC#C	Non_sub	Non_sub	Non_sub	anti-parkinsonian drug, treating early-stage parkinson's disease
Sulfasalazine	OC(=O)C1=C₩C(=N₩Nc2ccc(cc2)S(=O)(=O)Nc3ccccn3)₩C=CC1=O	Non_sub	Non_sub	Sub	synthetic peptide
Sumatriptan	CNS(=O)(=O)Cc1ccc2[nH]cc(CCN(C)C)c2c1	Non_sub	Non_sub	Non_sub	anti-inflammatory agent, treating inflammatory bowel disease, rheumatoid arthritis, enthesitis
Tacrine	Nc1c2CCCCc2nc3ccccc13	Non_sub	Non_sub	Non_sub	treating migraine headaches
Tamoxifen	CC₩C(=C(/c1ccccc1)₩c2ccc(OCCN(C)C)cc2)₩c3ccccc3	Non_sub	Sub	Sub	centrally-acting cholinesterase inhibitors

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
Testosterone	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O	Non_sub	Non_sub	Non_sub	antagonist of the estrogen receptor in breast tissue
Triamterene	Nc1nc(N)c2nc(c(N)nc2n1)c3ccccc3	Non_sub	Non_sub	Sub	steroid hormone
Triforine	ClC(Cl)(Cl)C(NC=O)N1CCN(CC1)C(NC=O)C(Cl)(Cl)Cl	Non_sub	Sub	Sub	potassium-sparcing diuretic, treating fluid retention and high blood pressure
Vinclozolin	CC1(OC(=O)N(C1=O)c2cc(Cl)cc(Cl)c2)C=C	Non_sub	Non_sub	Non_sub	pesticide
Warfarin	CC(=O)CC(C1=C(O)Oc2ccccc2C1=O)c3ccccc3	Non_sub	Non_sub	Non_sub	dicarboximide fungicide
Zimeldine	CN(C)C₩C=C(₩c1ccc(Br)cc1)/c2cccnc2	Non_sub	Sub	Non_sub	anticoagulant
Acebutolol	CCCC(=O)Nc1ccc(OCC(O)CNC(C)C)c(c1)C(=O)C	Sub	Sub	Sub	antihypertensive, antiarrhythmatic
Actinomycin	CC(C)C1NC(=O)C(NC(=O)C2=C(N)C(=O)C(=C3Oc4c(C)ccc(C(=O)NC5C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C6CCCN6C(=O)C(NC5=O)C(C)C)c4N=C23)C)C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C7CCCN7C1=O	Sub	Non_sub	Non_sub	polypeptide antibiotics
actinomycin_d	CC(C)C1NC(=O)C(NC(=O)C2=C(N)C(=O)C(=C3Oc4c(C)ccc(C(=O)NC5C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C6CCCN6C(=O)C(NC5=O)C(C)C)c4N=C23)C)C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C7CCCN7C1=O	Sub	Non_sub	Non_sub	actinomycin
adriamycin	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5C[C@H](N)[C@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)CO	Sub	Sub	Sub	antibiotic, anthracycline
Aldosterone	C[C@]12CCC(=O)C=C1CC[C@H]3[C@@	Sub	Sub	Sub	hormone

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	H]4CC[C@H](C(=O)CO)[C@]4(C[C@H](O)[C@H]23)C=O				
Amiodarone	CCCCc1oc2ccccc2c1C(=O)c3cc(I)c(OCCN(CC)CC)c(I)c3	Sub	Sub	Sub	antiarrhythmic
amoxicillin	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)c3ccc(O)cc3)C(=O)N2[C@H]1C(=O)O	Sub	Non_sub	Sub	antibiotic
Amprenavir	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)O[C@H]2CCOC2)S(=O)(=O)c3ccc(N)cc3	Sub	Sub	Sub	anti-HIV, protease inhibitor
Astemizole	COc1ccc(CCN2CCC(CC2)Nc3nc4ccccc4n3Cc5ccc(F)cc5)cc1	Sub	Sub	Sub	antihistamine
Azidopine	CCOC(=O)C1=C(C)NC(=C(C1c2ccccc2C(F)(F)F)C(=O)OCCNC(=O)c3ccc(cc3)N=[N+]=[N-])C	Sub	Sub	Sub	anti-HIV
Bepridil	CC(C)COC[C@H](CN(Cc1ccccc1)c2ccccc2)N3CCCC3	Sub	Sub	Sub	calcium channel blocker
Bisantrene	C1CN=C(N₩N=C₩c2c3ccccc3c(₩C=N₩NC4=NCCN4)c5ccccc25)N1	Sub	Sub	Sub	antitumour antibiotic
bunitrolol	CC(C)(C)NCC(O)COc1ccccc1C#N	Sub	Non_sub	Non_sub	antihypertensive
Calphostin	COC1=CC(=O)c2c(O)c(OC)c(CC(C)OC(=O)Oc3ccc(O)cc3)c4c2c1c5C(=CC(=O)c6c(O)c(OC)c(CC(C)OC(=O)c7ccccc7)c4c56)OC	Sub	Non_sub	Non_sub	protein kinase C inhibitor, natural product
catharanthine	CCC1=C[C@H]2CN3CCc4c([nH]c5ccccc45)[C@@](C2)([C@@H]13)C(=O)OC	Sub	Sub	Sub	stimulator of pancreatic enzyme
Cefazolin	Cc1nnc(SCC2=C(N3[C@H](SC2)[C@H](NC(=O)Cn4cnnn4)C3=O)C(=O)O)s1	Sub	Sub	Sub	antibiotic
Cefoperazone	CCN1CCN(C(=O)NC(C(=O)N[C@H]2[C@H]3SCC(=C(N3C2=O)C(=O)O)CSc4nn	Sub	Sub	Sub	cephalosporin antibiotic

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	nn4C)c5ccc(O)cc5)C(=O)C1=O				
Cefotetan	CO[C@]1(NC(=O)C2SC(=C(C(=O)N)C(=O)O)S2)C3SCC(=C(N3C1=O)C(=O)O)CSc4nnnn4C	Sub	Sub	Sub	antibiotic
Celiprolol	CCN(CC)C(=O)Nc1ccc(OCC(O)CNC(C)(C)C)c(c1)C(=O)C	Sub	Sub	Sub	antihypertensive
Cepharanthine	COc1ccc2C[C@H]3N(C)CCc4cc(OC)c(Oc5c6OCOc6cc7CCN(C)[C@@H](Cc8ccc(Oc1c2)cc8)c57)cc34	Sub	Sub	Sub	plant alkaloid, P-gp inhibitor
Chloroquine	CCN(CC)CCCC(C)Nc1ccnc2cc(Cl)ccc12	Sub	Sub	Sub	anti-malaria
Cimetidine	C₩N=C(₩NCCSCc1nc[nH]c1C)/NC#N	Sub	Non_sub	Sub	histamine H2-receptor antagonist
Cinchonidine	OC(C1CC2CCN1CC2C=C)c3ccnc4ccccc34	Sub	Non_sub	Sub	anti-malaria, antifebrile
ciprofloxacin	OC(=O)C1=CN(C2CC2)c3cc(N4CCNCC4)c(F)cc3C1=O	Sub	Sub	Sub	antibacterial
cis-flupenthixol	OCCN1CCN(CC₩C=C/2₩c3ccccc3Sc4ccc(cc24)C(F)(F)F)CC1	Sub	Sub	Sub	antipsychotic
clarithromycin	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]3O[C@H](C)C[C@@H]([C@H]3O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)OC	Sub	Sub	Sub	macrolide antibiotics
Clotrimazole	Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4	Sub	Non_sub	Non_sub	antifungal
Colchicine	COC1=CC=C2C(=CC1=O)[C@H](CCc3cc(OC)c(OC)c(OC)c23)NC(=O)C	Sub	Sub	Sub	anti-cancer
Corticosterone	C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C	Sub	Sub	Sub	hormone

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	@@H]2C(=O)CO				
cortisol	C[C@]12CCC(=O)C=C1CC[C@H]3[C@@H]4CC[C@](O)(C(=O)CO)[C@@]4(C)C[C@H](O)[C@H]23	Sub	Sub	Sub	hormone
CP100356	COc1ccc(CCNc2nc(N3CCc4cc(OC)c(OC)cc4C3)c5cc(OC)c(OC)cc5n2)cc1OC	Sub	Sub	Sub	P-gp inhibitor
Cyclosporin	CCC1NC(=O)C(C(O)C(C)C₩C=C₩C)N(C)C(=O)C(C(C)C)N(C)C(=O)C(CC(C)C)N(C)C(=O)C(CC(C)C)N(C)C(=O)C(C)NC(=O)C(C)NC(=O)C(CC(C)C)N(C)C(=O)C(NC(=O)C(CC(C)C)N(C)C(=O)CN(C)C1=O)C(C)C	Sub	Non_sub	Non_sub	immunosuppressant drug
Daunomycin	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5C[C@H](N)[C@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)C	Sub	Sub	Sub	anti-cancer, anti-leukemic
debrisoquine	NC(=N)N1CCc2ccccc2C1	Sub	Non_sub	Non_sub	antihypertensive
Dexamethasone	C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO	Sub	Sub	Sub	antiinflammatory
Dexniguldipine	CCCN1C(=C([C@H](C(=C1C)C(=O)ON2CCC(CC2)(c3ccccc3)c4ccccc4)c5cccc(c5)[N+](=O)[O-])C(=O)OC)C	Sub	Non_sub	Non_sub	inhibitor of human pancreatic adenocarinoma
Dibucaine	CCCCOc1cc(C(=O)NCCN(CC)CC)c2ccccc2n1	Sub	Sub	Sub	local anesthetic
Digitoxigenin	C[C@]12CC[C@H](O)C[C@H]1CC[C@@H]3[C@@H]2CC[C@]4(C)[C@H](CC[C@]34O)C5=CC(=O)OC5	Sub	Sub	Sub	toxin
Digitoxin	C[C@H]1O[C@H](C[C@H](O)[C@@H]1O)O[C@H]2[C@@H](O)C[C@H](O[C@H]3[C@@H](O)C[C@H](O[C@H]4CC[C@	Sub	Sub	Sub	toxin

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	@]5(C)[C@H](CC[C@@H]6[C@@H]5CC[C@]7(C)[C@H](CC[C@]67O)C8=CC(=O)OC8)C4)O[C@@H]3C)O[C@@H]2C				
Digoxigenin	C[C@]12CC[C@H](O)C[C@H]1CC[C@@H]3[C@@H]2C[C@@H](O)[C@]4(C)[C@H](CC[C@]34O)C5=CC(=O)OC5	Sub	Sub	Sub	hapten
Digoxin	C[C@H]1O[C@H](C[C@H](O)[C@@H]1O)O[C@H]2[C@@H](O)C[C@H](O[C@H]3[C@@H](O)C[C@H](O[C@H]4CC[C@@]5(C)[C@H](CC[C@@H]6[C@@H]5C[C@@H](O)[C@]7(C)C(CC[C@]67O)C8=CC(=O)OC8)C4)O[C@@H]3C)O[C@@H]2C	Sub	Sub	Sub	treatment of various heart condition
Dipyridamole	OCCN(CCO)c1nc(N2CCCCC2)c3nc(nc(N4CCCCC4)c3n1)N(CCO)CCO	Sub	Non_sub	Sub	anti-thrombus formation
Docetaxel	CC(=O)O[C@@]12CO[C@@H]1C[C@H](O)[C@]3(C)[C@@H]2[C@H](OC(=O)c4ccccc4)[C@]5(O)C[C@H](OC(=O)[C@H](O)[C@@H](NC(=O)OC(C)(C)C)c6ccccc6)C(=C([C@@H](O)C3=O)C5(C)C)C	Sub	Sub	Sub	anti-mitotic chemotherapy drug
Domperidone	Clc1ccc2N(C3CCN(CCCN4C(=O)Nc5ccccc45)CC3)C(=O)Nc2c1	Sub	Sub	Sub	antidopaminergic
efavirenz	FC(F)(F)[C@]1(OC(=O)Nc2ccc(Cl)cc12)C#CC3CC3	Sub	Sub	Sub	non-nucleonon-nucleoside reverse transcriptase inhibitor
eletriptan	CN1CCC[C@@H]1Cc2c[nH]c3ccc(CCS(=O)(=O)c4ccccc4)cc23	Sub	Sub	Sub	antimigraine
Emetine	CC[C@H]1CN2CCc3cc(OC)c(OC)cc3[C@@H]2C[C@@H]1C[C@H]4NCCc5cc(OC)c(OC)cc45	Sub	Sub	Sub	anti-protozoal
Endosulfan	ClC1=C(Cl)C2(Cl)C3COS(=O)OCC3C1(Cl)	Sub	Non_sub	Non_sub	insecticide

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	C2(Cl)Cl				
enoxacin	CCN1C=C(C(=O)O)C(=O)c2cc(F)c(nc12)N3CCNCC3	Sub	Sub	Sub	antibacterial
epirubicin	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5C[C@H](N)[C@@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)CO	Sub	Sub	Sub	antibiotic, anthracycline
epothilone_a	C[C@H]1CCC[C@H]2O[C@H]2C[C@H](OC(=O)C[C@H](O)C(C)(C)C(=O)[C@H](C)[C@H]1O)₩C(=C₩c3csc(C)n3)₩C	Sub	Sub	Sub	anti-cancer
Erythromycin	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]3O[C@H](C)C[C@@H]([C@H]3O)N(C)C)[C@](C)(O)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O	Sub	Sub	Sub	macrolide antibiotics
estradiol	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O	Sub	Non_sub	Non_sub	a sex hormone
Estriol	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](O)[C@@H]2O	Sub	Non_sub	Non_sub	one of the three main estrogen
Etoposide	COc1cc(cc(OC)c1O)[C@H]2[C@@H]3[C@H](COC3=O)[C@H](O[C@@H]4O[C@@H]5CO[C@@H](C)O[C@H]5[C@H](O)[C@H]4O)c6cc7OCOc7cc26	Sub	Sub	Sub	anti-cancer, topoisomerase 2 inhibitor
fexofenadine	CC(C)(C(=O)O)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4	Sub	Sub	Sub	antihistamine
flunitrazepam	CN1C(=O)CN=C(c2ccccc2F)c3cc(ccc13)[N+](=O)[O-]	Sub	Non_sub	Non_sub	anticonvulsant
Fluphenazine	OCCN1CCN(CCCN2c3ccccc3Sc4ccc(cc24)C(F)(F)F)CC1	Sub	Sub	Sub	antipsychotic

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
Gallopamil	COc1ccc(CCN(C)CCCC(C#N)(C(C)C)c2cc(OC)c(OC)c(OC)c2)cc1OC	Sub	Sub	Sub	anti-arrythmic
haloperidol	OC1(CCN(CCCC(=O)c2ccc(F)cc2)CC1)c3ccc(Cl)cc3	Sub	Sub	Sub	antipsychotic
Hydrocortisone	C[C@]12CCC(=O)C=C1CC[C@H]3[C@@H]4CC[C@](O)(C(=O)CO)[C@@]4(C)C[C@H](O)[C@H]23	Sub	Sub	Sub	hormone
Hydroxyrubicin	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5CC(O)[C@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)CO	Sub	Sub	Sub	anti-cancer, topoisomerase 1 inhibitor
Idarubicin	C[C@@H]1O[C@H](C[C@H](N)[C@@H]1O)O[C@H]2C[C@@](O)(Cc3c(O)c4C(=O)c5ccccc5C(=O)c4c(O)c23)C(=O)C	Sub	Non_sub	Sub	anti-leukemic
Indinavir	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	Sub	Sub	Sub	highly active antiretroviral drug, protease inhibitor
irinotecan	CCc1c2CN3C(=O)C4=C(C=C3c2nc5ccc(OC(=O)N6CCC(CC6)N7CCCCC7)cc15)[C@@](O)(CC)C(=O)OC4	Sub	Sub	Sub	anti-cancer, topoisomerase 1 inhibitor
Isosafrole	C₩C=C₩c1ccc2OCOc2c1	Sub	Non_sub	Non_sub	psychoactive drug MDMA ('ecstasy')
Ivermectin	CCC(C)C1O[C@]2(CCC1C)C[C@@H]3CC(C₩C=C(/C)₩C(O[C@H]4C[C@H](OC)C(O[C@H]5C[C@H](OC)C(O)[C@H](C)O5)[C@H](C)O4)C(C)₩C=C₩C=C₩6/COC7[C@H](O)C(=C[C@@H](C(=O)O3)C67O)C)O2	Sub	Sub	Sub	antiparasitic avermectin drug
k02	CCN(CC)C(=O)c1c2C[C@H](C)CCc2sc1NC(=O)c3cccs3	Sub	Sub	Sub	cystein protease inhibitor

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
L_dopa	N[C@@H](Cc1ccc(O)c(O)c1)C(=O)O	Sub	Non_sub	Non_sub	psychoactive drug
Leupeptin	CC(C)C[C@H](NC(CCCN=C(N)N)C=O)C(=O)NC(=O)[C@H](CC(C)C)NC(=O)C	Sub	Non_sub	Sub	protease inhibitor
levofloxacin	C[C@H]1COc2c(N3CCN(C)CC3)c(F)cc4C(=O)C(=CN1c24)C(=O)O	Sub	Sub	Sub	antibiotic
Levomeprazine	COc1ccc2Sc3ccccc3N(CC(C)CN(C)C)c2c1	Sub	Sub	Sub	histamine-antagonist properties of the antihistamines
Loperamide	CN(C)C(=O)C(CCN1CCC(O)(CC1)c2ccc(Cl)cc2)(c3ccccc3)c4ccccc4	Sub	Sub	Sub	anti-diarrhea, opioid drug
loratidine	CCOC(=O)N1CCC(=C2c3ccc(Cl)cc3CCc4cccnc24)CC1	Sub	Non_sub	Non_sub	antihistamine
losartan	CCCCc1nc(Cl)c(CO)n1Cc2ccc(cc2)c3ccccc3c4nn[nH]n4	Sub	Sub	Sub	antihypertensive
Lovastatin	CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@@H]12	Sub	Sub	Sub	lowering cholesterol, anti-cadiovascular disease
LY335979	O[C@@H](COc1cccc2ncccc12)CN3CCN(CC3)C4c5ccccc5[C@H]6[C@@H](c7ccccc47)C6(F)F	Sub	Sub	Sub	Antineoplastic Agents
Mequitazine	C(C1CN2CCC1CC2)N3c4ccccc4Sc5ccccc35	Sub	Sub	Sub	anhihistamine, anticholinergic
Methadone	CCC(=O)C(CC(C)N(C)C)(c1ccccc1)c2ccccc2	Sub	Sub	Sub	narcotic pain reliever
Methylprednisolone	C[C@H]1C[C@H]2[C@@H]3CC[C@](O)(C(=O)CO)[C@@]3(C)C[C@H](O)[C@@H]2[C@@]4(C)C=CC(=O)C=C14	Sub	Sub	Sub	anti-inflammatory
Methylreserpate	CCOC(=O)Oc1c(OC)cc(cc1OC)C(=O)O[C@@H]2C[C@@H]3CN4CCc5c([nH]c6cc(OC)ccc56)[C@H]4C[C@@H]3[C@@H]([	Sub	Sub	Sub	antihypertensive

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	C@H]2OC)C(=O)OC				
mithramycin	CO[C@@H]([C@@H]1Cc2cc3cc(O[C@H]4C[C@@H](O[C@H]5C[C@@H](O)[C@H](O)[C@@H](C)O5)[C@H](O)[C@@H](C)O4)c(C)c(O)c3c(O)c2C(=O)[C@H]1O[C@H]6C[C@@H](O[C@H]7C[C@@H](O[C@H]8C[C@](C)(O)[C@H](O)[C@@H](C)O8)[C@@H](O)[C@@H](C)O7)[C@H](O)[C@@H](C)O6)C(=O)[C@@H](O)[C@@H](C)O	Sub	Non_sub	Non_sub	antineoplastic antibiotics
mitomycin	CO[C@]12[C@H]3N[C@H]3CN1C4=C([C@H]2COC(=O)N)C(=O)C(=C(C)C4=O)N	Sub	Sub	Non_sub	antitumour antibiotic
Mitoxantrone	OCCNCCNc1ccc(NCCNCCO)c2C(=O)c3c(O)ccc(O)c3C(=O)c12	Sub	Non_sub	Non_sub	Antineoplastic Agents
Monensin	CC[C@]1(CC[C@@H](O1)[C@@]2(C)CC[C@]3(C[C@H](O)[C@@H](C)[C@H](O3)[C@H](C)[C@H](OC)[C@@H](C)C(=O)O)O2)[C@H]4O[C@@H](C[C@H]4C)[C@H]5O[C@@](O)(CO)[C@H](C)C[C@@H]5C	Sub	Sub	Sub	polyether ionophore antibiotics
Morphine	CN1CC[C@]23[C@H]4Oc5c(O)ccc(C[C@@H]1[C@@H]2C=C[C@@H]4O)c35	Sub	Non_sub	Non_sub	potent opiate analgesic
morphine-6-glucuronide	CN1CC[C@]23[C@H]4Oc5c(O)ccc(C[C@@H]1[C@@H]2C=C[C@@H]4O[C@@H]6O[C@@H]([C@@H](O)[C@H](O)[C@H]6O)C(=O)O)c35	Sub	Non_sub	Sub	metabolite of morphine, pain-relieving
m-prednisolone	C[C@H]1C[C@H]2[C@@H]3CC[C@](O)(C(=O)CO)[C@@]3(C)C[C@H](O)[C@@H	Sub	Sub	Sub	anti-inflammatory

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	]2[C@@]4(C)C=CC(=O)C=C14				
navelbine	CCC1=CC2CN(C1)Cc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](OC(=O)C)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)OC	Sub	Sub	Sub	vinorelbine
nefazodone	CCC1=NN(CCCN2CCN(CC2)c3cccc(Cl)c3)C(=O)N1CCOc4ccccc4	Sub	Sub	Sub	antidepressant
Nelfinavir	Cc1c(O)cccc1C(=O)N[C@@H](CSc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	Sub	Sub	Sub	anti-HIV, antiretroviral
nevirapine	Cc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12	Sub	Non_sub	Non_sub	an antiretroviral drug
Nimodipine	COCCOC(=O)C1=C(C)NC(=C(C1c2cccc(c2)[N+](=O)[O-])C(=O)OC(C)C)C	Sub	Sub	Sub	antihypertensive
nortriptyline	CNCCC=C1c2ccccc2CCc3ccccc13	Sub	Non_sub	Non_sub	antidepressant (TCA)
NSC328426	CC1COC2(CC1OC(=O)₩C=C₩c3ccccc3)OC4CC(CCC4C25CO5)C(=O)OC6OC(C)C(O)C(OC(=O)C)C6OC7OC(C)C(O)C(OC(=O)C)C7O	Sub	Sub	Sub	anti-cancer
NSC339281	CC(C)C1NC(=O)C(NC(=O)c2ccc(C)c3Oc4c(C)c5OC(=O)C(=Nc5c(C(=O)NC6C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C7CCCN7C(=O)C(NC6=O)C(C)C)c4Nc23)c8ccccc8)C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C9CCCN9C1=O	Sub	Non_sub	Non_sub	-
NSC359449	CCN(CC)CC[n+]1ccc2c(C)c3[nH]c4ccccc4c3c(C)c2c1	Sub	Sub	Sub	anti-tumor
NSC630176	C₩C=C₩1/NC(=O)[C@H]2CSSCC₩C=C₩[C@H](CC(=O)N[C@H](C(C)C)C(=O)N	Sub	Non_sub	Sub	HDAC inhibitor

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	2)OC(=O)[C@@H](NC1=O)C(C)C				
NSC640085	CC[n+]1c(₩C=C₩c2ccc(cc2)N(CCCl)CCCl)ccc3cc(NC(=O)₩C=C₩c4ccccc4)ccc13	Sub	Sub	Sub	-
NSC66490	CN1CCC=CC1	Sub	Non_sub	Non_sub	-
Ondansetron	Cc1nccn1CC2CCc3c(C2=O)c4ccccc4n3C	Sub	Non_sub	Sub	a serotonin 5-HT_3 receptor antagonist
Paclitaxel	CC(=O)O[C@H]1C(=O)[C@]2(C)[C@@H](O)C[C@H]3OC[C@@]3(OC(=O)C)[C@H]2[C@H](OC(=O)c4ccccc4)[C@]5(O)C[C@H](OC(=O)[C@H](O)[C@@H](NC(=O)c6ccccc6)c7ccccc7)C(=C1C5(C)C)C	Sub	Sub	Sub	anti-mitotic chemotherapy drug
Pafenolol	CC(C)NCC(O)COc1ccc(CCNC(=O)NC(C)C)cc1	Sub	Sub	Sub	beta-1-andrenoceptor antagonist
pararosaniline	Nc1ccc(cc1)C(=C2C=CC(=N)C=C2)c3ccc(N)cc3	Sub	Non_sub	Non_sub	a single dye, may make the best Schiff's reagent
Perphenazine	OCCN1CCN(CCCN2c3ccccc3Sc4ccc(Cl)cc24)CC1	Sub	Sub	Sub	antipsychotic
Phenobarbital	CCC1(C(=O)NC(=O)NC1=O)c2ccccc2	Sub	Non_sub	Non_sub	anticonvulsant
Phenoxazine	N1c2ccccc2Oc3ccccc13	Sub	Non_sub	Non_sub	chromophore of actinomycin antibiotics
Phenytoin	O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3	Sub	Non_sub	Non_sub	antiepileptic
Pimozide	Fc1ccc(cc1)C(CCCN2CCC(CC2)N3C(=O)Nc4ccccc34)c5ccc(F)cc5	Sub	Sub	Sub	antipsychotic
Prazosin	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)c4occc4	Sub	Sub	Sub	antihypertensive
promazine	CN(C)CCCN1c2ccccc2Sc3ccccc13	Sub	Non_sub	Non_sub	antipsychotic
Protriptyline	CNCCCC1c2ccccc2C=Cc3ccccc13	Sub	Non_sub	Non_sub	a tricyclic antidepressant (TCA)
Puromycin	COc1ccc(C[C@H](N)C(=O)NC2C(CO)OC(C2O)n3cnc4c(ncnc34)N(C)C)cc1	Sub	Non_sub	Sub	antibiotic
Quinidine	COc1ccc2nccc([C@H](O)[C@H]3C[C@@H]4CCN3C[C@@H]4C=C)c2c1	Sub	Sub	Sub	class I antiarrhythmic

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
Quinine	COc1ccc2nccc([C@@H](O)[C@@H]3CC4CCN3C[C@@H]4C=C)c2c1	Sub	Sub	Sub	antipyretic
Rapamycin	CO[C@@H]1C[C@H](C[C@@H](C)[C@@H]2CC(=O)[C@H](C)₩C=C(/C)₩[C@@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)₩C=C/C=C/C=C(₩C)/[C@H](C[C@@H]3CC[C@@H](C)[C@@](O)(O3)C(=O)C(=O)N4CCCC[C@H]4C(=O)O2)OC)CC[C@H]1O	Sub	Sub	Sub	immunosuppressant drug
Reserpine	CO[C@H]1[C@@H](C[C@@H]2CN3CCc4c([nH]c5cc(OC)ccc45)[C@H]3C[C@@H]2[C@@H]1C(=O)OC)OC(=O)c6cc(OC)c(OC)c(OC)c6	Sub	Sub	Sub	antipsychotic, antihypertensive
Rhodamine	COC(=O)c1ccccc1C2=C3C=CC(=[NH2+])C=C3Oc4cc(N)ccc24	Sub	Non_sub	Non_sub	dye
Rifampicin	CO[C@H]1₩C=C₩O[C@@]2(C)Oc3c(C)c(O)c4C(=C(NC(=O)₩C(=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(=O)C)[C@@H]1C)₩C)₩C(=C/NN5CCN(C)CC5)₩C(=O)c4c3C2=O)O	Sub	Sub	Non_sub	bactericidal antibiotics
Risperidone	CC1=C(CCN2CCC(CC2)c3noc4cc(F)ccc34)C(=O)N5CCCCC5=N1	Sub	Sub	Sub	antipsychotic
Ritonavir	CC(C)[C@H](NC(=O)N(C)Cc1csc(n1)C(C)C)C(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3cncs3)Cc4ccccc4	Sub	Non_sub	Sub	antiretroviral drug
S9788	Fc1ccc(cc1)C(CNC2CCN(CC2)c3nc(NCC=C)nc(NCC=C)n3)c4ccc(F)cc4	Sub	Sub	Sub	Antineoplastic Agents
Safingol	CCCCCCCCCCCCCCC[C@@H](O)[C@@H	Sub	Non_sub	Sub	a lyso-sphingolipid protein kinase C inhibitor

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	](N)CO				
Saquinavir	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4	Sub	Non_sub	Sub	antiretroviral drug
S-Farnesyl	CC(=CCC₩C(=C₩CC₩C(=C₩CSC[C@H](N)C(=O)O)₩C)₩C)C	Sub	Non_sub	Non_sub	antibiotic
sparfloxacin	C[C@@H]1CN(C[C@H](C)N1)c2c(F)c(N)c3C(=O)C(=CN(C4CC4)c3c2F)C(=O)O	Sub	Sub	Sub	psychoactive drug
Spiperone	Fc1ccc(cc1)C(=O)CCCN2CCC3(CC2)N(CNC3=O)c4ccccc4	Sub	Sub	Sub	anti-fungal, anti-hypertensive
Staurosporine	CN[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n3c4ccccc4c5c6CNC(=O)c6c7c8ccccc8n2c7c35	Sub	Sub	Sub	immunosuppressant drug
Tacrolimus	CO[C@@H]1CC(CC[C@H]1O)₩C=C(/C)₩[C@H]2OC(=O)[C@@H]3CCCCN3C(=O)C(=O)[C@]4(O)O[C@H]([C@H](C[C@@H](C)C₩C(=C₩[C@@H](CC=C)C(=O)C[C@H](O)[C@H]2C)₩C)OC)[C@H](C[C@H]4C)OC	Sub	Sub	Non_sub	beta-blocker
talinolol	CC(C)(C)NCC(O)COc1ccc(NC(=O)NC2CCCCC2)cc1	Sub	Sub	Sub	Paclitaxel
taxol	CC(=O)O[C@H]1C(=O)[C@]2(C)[C@@H](O)C[C@H]3OC[C@@]3(OC(=O)C)[C@H]2[C@H](OC(=O)c4ccccc4)[C@]5(O)C[C@H](OC(=O)[C@H](O)[C@@H](NC(=O)c6ccccc6)c7ccccc7)C(=C1C5(C)C)C	Sub	Sub	Sub	anti-cancer, topoisomerase 2 inhibitor
Teniposide	COc1cc(cc(OC)c1O)[C@H]2[C@@H]3[C@H](COC3=O)[C@H](O[C@@H]4O[C@	Sub	Sub	Sub	antihistamine

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	@H]5CO[C@H](O[C@H]5[C@H](O)[C@H]4O)c6cccs6)c7cc8OCOc8cc27				
Terfenadine	CC(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4	Sub	Sub	Sub	Antineoplastic Agents
tetraphenylphosphonium	c1ccc(cc1)[P+](c2ccccc2)(c3ccccc3)c4ccccc4	Sub	Non_sub	Non_sub	antipsychotic
Thioridazine	CSc1ccc2Sc3ccccc3N(CCC4CCCCN4C)c2c1	Sub	Sub	Sub	anti-cancer
Topotecan	CC[C@@]1(O)C(=O)OCC2=C1C=C3N(Cc4cc5c(CN(C)C)c(O)ccc5nc34)C2=O	Sub	Sub	Sub	anti-cancer
Toremifene	CN(C)CCOc1ccc(cc1)₩C(=C(₩CCCl)/c2ccccc2)₩c3ccccc3	Sub	Sub	Sub	antidepressant
trazodone	Clc1cccc(c1)N2CCN(CCCN3N=C4C=CC=CN4C3=O)CC2	Sub	Sub	Sub	antipsychotic
Trifluoperazine	CN1CCN(CCCN2c3ccccc3Sc4ccc(cc24)C(F)(F)F)CC1	Sub	Sub	Sub	antipsychotic
Triflupromazine	CN(C)CCCN1c2ccccc2Sc3ccc(cc13)C(F)(F)F	Sub	Sub	Sub	antimicrobial
Trimethoprim	COc1cc(Cc2cnc(N)nc2N)cc(OC)c1OC	Sub	Non_sub	Sub	potent agent against severe acute respiratory-syndrome coronavirus
Valinomycin	CC(C)C1NC(=O)C(C)OC(=O)C(NC(=O)C(OC(=O)C(NC(=O)C(C)OC(=O)C(NC(=O)C(OC(=O)C(NC(=O)C(C)OC(=O)C(NC(=O)C(OC1=O)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C	Sub	Non_sub	Non_sub	antimicrotubule drug, anti-cancer
Vinblastine	CC[C@]1(O)C[C@@H]2CN(CCc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](OC(=O)C)[C@]8(CC)C=CCN9CC[C@]67[C@H]	Sub	Sub	Sub	anti-mitotic chemotherapy drug

Name	Smiles	Class	Predicted Class_2D	Predicted Class_3D	Category or functions
	89)C(=O)OC)C1				
Vincristine	CC[C@]1(O)C[C@H]2CN(CCc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C=O)[C@H]7[C@](O)([C@H](OC(=O)C)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)OC)C1	Sub	Sub	Sub	anti-mitotic in leukeamia, lymphoma, melanoma, breast cancer
vindesine	CC[C@]1(O)C[C@H]2CN(CCc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](O)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)N)C1	Sub	Non_sub	Sub	anti-HIV
Vindoline	CCC12C=CCN3CC[C@@]4([C@H]13)[C@@H](N(C)c5cc(OC)ccc45)[C@](O)([C@@H]2OC(=O)C)C(=O)OC	Sub	Sub	Sub	anti-mitotic chemotherapy drug
vinorelbine	CCC1=CC2CN(C1)Cc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](OC(=O)C)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)OC	Sub	Sub	Sub	antihypertensive, antiarrhythmatic

Table S2. Description of molecular descriptors used in 2D and 3D RP models

Molecular descriptors	Meaning
Molecular_weight (MW)	Molecular weight calculated in descriptor calculation module in PreADMET 2.0
No_H_bond_donors (No_HB_Donor)	Number of atoms that can be used as hydrogen bond donors
No_H_bond_acceptors	Number of atoms that can be used as hydrogen bond acceptors
Topological_PSA	Molecular polar surface area based on surface contribution of polar fragments
C_PSA	Molecular polar surface area based on exposed surface area of polar atoms on Connolly surface
SFED_logP	logP based on Solvation Free Energy Density models

Table S3. Summary of results from SVM classifications using descriptors in 2D and 3D RP models

	Using 2D descriptors	Using 3D descriptors
Accuracy	0.815	0.796
Sensitivity	0.857	0.850
Specificity	0.763	0.727

Table S4. Overall results from SVM classifications of Table S3

Name	Smiles	class	SVM_2D _pred.	SVM_3D _pred.
Aldicarb	CNC(=O)O₩N=C₩C(C)(C)SC	Non_sub	Non_sub	Non_sub
Aldoxycarb	CNC(=O)O₩N=C₩C(C)(C)S(=O)(=O)C	Non_sub	Non_sub	Non_sub
Amantadine	NC12CC3CC(CC(C3)C1)C2	Non_sub	Non_sub	Non_sub
Aminocarb	CNC(=O)Oc1ccc(N(C)C)c(C)c1	Non_sub	Non_sub	Non_sub
Antipyrine	CN1N(C(=O)C=C1C)c2ccccc2	Non_sub	Non_sub	Non_sub
Atenolol	CC(C)NCC(O)COc1ccc(CC(=O)N)cc1	Non_sub	Non_sub	Non_sub
Atrazine	CCNc1nc(Cl)nc(NC(C)C)n1	Non_sub	Non_sub	Non_sub
BIBW22	C[C@@H]1CN(C[C@H](C)O1)c2nc(N(CCO)CC(C)(C)O)c3nc(c4ccccc4)c(nc3n2)N5C[C@@H](C)O[C@@H](C)C5	Non_sub	sub	sub
Biperiden	OC(CCN1CCCCC1)(C2CC3CC2C=C3)c4ccccc4	Non_sub	sub	sub
Carbaryl	CNC(=O)Oc1cccc2ccccc12	Non_sub	Non_sub	Non_sub

Carboplatin	OC(=O)C1(CCC1)C(=O)O	Non_sub	Non_sub	Non_sub
Carmustine	ClCCNC(=O)N(CCCl)N=O	Non_sub	Non_sub	Non_sub
Chaps	C[C@H](CCC(=O)NCCC[N+](C)(C)CCCS(=O)(=O)[O-])[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C	Non_sub	sub	sub
Chlorambucil	OC(=O)CCCc1ccc(cc1)N(CCCl)CCCl	Non_sub	Non_sub	Non_sub
Chlorpheniramine	CN(C)CCC(c1ccc(Cl)cc1)c2ccccn2	Non_sub	Non_sub	Non_sub
Clonidine	Clc1cccc(Cl)c1NC2=NCCN2	Non_sub	sub	sub
Cortexolone	C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@H]2CC[C@@]4(C)[C@H]3CC[C@]4(O)C(=O)CO	Non_sub	sub	sub
Cyclophosphamide	ClCCN(CCCl)P1(=O)NCCCO1	Non_sub	Non_sub	Non_sub
Cytarabine	NC1=NC(=O)N(C=C1)[C@@H]2O[C@H](CO)[C@@H](O)[C@@H]2O	Non_sub	Non_sub	Non_sub
Deoxycorticosterone	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2C(=O)CO	Non_sub	sub	Non_sub
deoxypodophyllotoxin	COc1cc(cc(OC)c1OC)[C@H]2[C@@H]3[C@H](COC3=O)Cc4cc5OCOc5cc24	Non_sub	Non_sub	Non_sub
Dialifos	CCOP(=S)(OCC)SC(CCl)N1C(=O)c2ccccc2C1=O	Non_sub	Non_sub	Non_sub
Dieldrin	ClC1=C(Cl)[C@]2(Cl)C3[C@H]4C[C@H](C5OC45)C3[C@]1(Cl)C2(Cl)Cl	Non_sub	Non_sub	Non_sub
Doxylamine	CN(C)CCOC(C)(c1ccccc1)c2ccccn2	Non_sub	Non_sub	Non_sub
Epinephrine	CNC[C@H](O)c1ccc(O)c(O)c1	Non_sub	Non_sub	Non_sub
Epipodophyllotoxin	COc1cc(cc(OC)c1OC)[C@H]2[C@@H]3[C@H](COC3=O)[C@H](O)c4cc5OCOc5cc24	Non_sub	sub	Non_sub
fluazifop-butyl	CCCCOC(=O)C(C)Oc1ccc(Oc2ccc(cn2)C(F)(F)F)cc1	Non_sub	Non_sub	Non_sub
Flumazenil	CCOC(=O)c1ncn2c1CN(C)C(=O)c3cc(F)ccc23	Non_sub	Non_sub	Non_sub
Fluorouracil	FC1=CNC(=O)NC1=O	Non_sub	Non_sub	Non_sub
Guanabenz	NC(=N₩N=C₩c1c(Cl)cccc1Cl)N	Non_sub	Non_sub	Non_sub
Guanfacine	NC(=NC(=O)Cc1c(Cl)cccc1Cl)N	Non_sub	Non_sub	Non_sub
Imipramine	CN(C)CCCN1c2ccccc2CCc3ccccc13	Non_sub	Non_sub	sub
Indomethacin	COc1ccc2c(c1)c(CC(=O)O)c(C)n2C(=O)c3ccc(Cl)cc3	Non_sub	Non_sub	Non_sub
Itraconazole	CCC(C)N1N=CN(C1=O)c2ccc(cc2)N3CCN(CC3)c4ccc(OC[C@H]5CO[C@@](Cn6cncn6)(O5)c7ccc(Cl)cc7Cl)cc4	Non_sub	Non_sub	Non_sub
Ketamine	CNC1(CCCCC1=O)c2ccccc2Cl	Non_sub	Non_sub	Non_sub
Ketoconazole	CC(=O)N1CCN(CC1)c2ccc(OC[C@H]3CO[C@@](Cn4ccnc4)(O3)c5ccc(Cl)cc5Cl)cc2	Non_sub	Non_sub	Non_sub
Leptophos	COP(=S)(Oc1cc(Cl)c(Br)cc1Cl)c2ccccc2	Non_sub	Non_sub	Non_sub
Lidocaine	CCN(CC)CC(=O)Nc1c(C)cccc1C	Non_sub	Non_sub	sub

Lindane	ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	Non_sub	Non_sub	Non_sub
Mannitol	OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	Non_sub	Non_sub	Non_sub
Mebendazole	COC(=O)Nc1nc2ccc(cc2[nH]1)C(=O)c3ccccc3	Non_sub	Non_sub	sub
Mephentermine	CNC(C)(C)Cc1ccccc1	Non_sub	Non_sub	Non_sub
Meprobamate	CCCC(C)(COC(=O)N)COC(=O)N	Non_sub	Non_sub	Non_sub
Methoxychlor	COc1ccc(cc1)C(c2ccc(OC)cc2)C(Cl)(Cl)Cl	Non_sub	Non_sub	Non_sub
Metoprolol	COCCc1ccc(OCC(O)CNC(C)C)cc1	Non_sub	Non_sub	Non_sub
Mevinphos	COC(=O)₩C=C(/C)₩OP(=O)(OC)OC	Non_sub	Non_sub	Non_sub
Mexiletine	CC(N)COc1c(C)cccc1C	Non_sub	Non_sub	Non_sub
Midazolam	Cc1ncc2CN=C(c3ccccc3F)c4cc(Cl)ccc4n12	Non_sub	Non_sub	Non_sub
Mirex	ClC1(Cl)C2(Cl)C3(Cl)C4(Cl)C(Cl)(Cl)C5(Cl)C(Cl)(C1(Cl)C35Cl)C24Cl	Non_sub	Non_sub	sub
Naloxone	Oc1ccc2C[C@H]3N(CC=C)CC[C@@]45[C@@H](Oc1c24)C(=O)CC[C@@]35O	Non_sub	sub	sub
Naltrexone	Oc1ccc2C[C@H]3N(CC4CC4)CC[C@@]56[C@@H](Oc1c25)C(=O)CC[C@@]36O	Non_sub	sub	sub
Nigericin	CO[C@@H]1C[C@@H](C[C@H]2CC[C@H](C)[C@@H](O2)[C@@H](C)C(=O)O)O[C@]3(O[C@@](C)(C[C@H]3C)[C@H]4CC[C@](C)(O4)[C@@H]5O[C@H](C[C@@H]5C)[C@H]6O[C@@](O)(CO)[C@H](C)C[C@@H]6C)[C@@H]1C	Non_sub	sub	sub
Nitrazepam	[O-][N+](=O)c1ccc2NC(=O)CN=C(c3ccccc3)c2c1	Non_sub	Non_sub	Non_sub
Nitrendipine	CCOC(=O)C1=C(C)NC(=C(C1c2cccc(c2)[N+](=O)[O-])C(=O)OC)C	Non_sub	Non_sub	Non_sub
Nordazepam	Clc1ccc2NC(=O)CN=C(c3ccccc3)c2c1	Non_sub	Non_sub	Non_sub
NSC268251	CC(C)CCCCCCCCCCCCC(=O)NCC(=O)NC1C(C)OC(Nc2ncnc3nc[nH]c23)C(O)C1O	Non_sub	sub	sub
NSC309132	OCC1OC(C(O)C1O)N2C=CC=NC2=O	Non_sub	Non_sub	Non_sub
NSC314622	COc1cc2C(=O)N(C)C3=C(C(=O)c4cc5OCOc5cc34)c2cc1OC	Non_sub	Non_sub	Non_sub
NSC364080	CC1C(N(C)C(C(C)C1=O)c2ccccc2)c3ccccc3	Non_sub	Non_sub	Non_sub
NSC49899	CCOC(=O)C1C(N(C)C(C(C(=O)OCC)C1=O)c2ccccc2)c3ccccc3	Non_sub	sub	sub
NSC606532	COc1cc(c(cc1N)[N+](=O)[O-])[N+](=O)[O-]	Non_sub	Non_sub	Non_sub
NSC615985	CC(C)OC(=O)c1cc(NC(=O)C2=C(C)OCCS2)ccc1Cl	Non_sub	sub	Non_sub
NSC617286	O=C(OCc1ccccc1)OOC(=O)OCc2ccccc2	Non_sub	Non_sub	Non_sub
NSC623083	COc1ccccc1NS(=O)(=O)c2cc(ccc2OCCOc3ccc(cc3S(=O)(=O)Nc4ccccc4OC)C(C)(C)C)C(C)(C)C	Non_sub	sub	sub
NSC630148	CC(C)C(=O)NC(C)C(=O)N(Cc1ccc2ccccc2c1)N=O	Non_sub	Non_sub	Non_sub
NSC630357	CC(C(=NNC(=O)c1c(O)ccc2ccccc12)CCC(=O)Nc3cc(C)ccc3C)C(=O)c4ccc(O)cc4	Non_sub	sub	sub

NSC630721	Cc1cc(C)nc(NS(=O)(=O)c2ccc(NC(=O)COC(=O)c3cccc4C(=O)c5ccccc5Nc34)cc2)n1	Non_sub	sub	sub
NSC633528	CN(C)CCCCN1CCc2c(C1=O)n(C)c3ccccc23	Non_sub	Non_sub	sub
NSC639677	Clc1ccccc1CN2N=C3C=CC=CC3=CC2=O	Non_sub	Non_sub	Non_sub
NSC648403	CS(=O)(=O)c1c(N)c2nc(Cl)cn2c3nc4ccccc4nc13	Non_sub	Non_sub	Non_sub
NSC653278	COc1ccc(cc1)C(=O)C(C(=O)c2ccc(OC)cc2)c3c(C(=O)c4ccc(OC)cc4)c5ccccc5n3C(=O)c6ccc(OC)cc6	Non_sub	Non_sub	Non_sub
NSC664565	CC1C=C(C)c2ccccc2N(CC3=NCCN3)C1C	Non_sub	sub	sub
NSC666331	CC1=CC(=C(C#N)C(=S)N1C2OC(CO)C(O)C(O)C2O)c3occc3	Non_sub	Non_sub	sub
NSC667532	OC[C@@H]1O[C@@H]([C@@H](O)[C@@H](O)C1O)N2C3=C(CCCC3)C(=C(C#N)C2=S)c4occc4	Non_sub	Non_sub	sub
NSC667533	CCOC(=O)C1=C(C)N(C2OC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C2OC(=O)C)C(=S)C(=C1c3ccc(Cl)cc3)C#N	Non_sub	Non_sub	Non_sub
NSC667551	CC(=O)C1=C(C)N(C2OC(CO)C(O)C(O)C2O)C(=S)C(=C1c3occc3)C#N	Non_sub	Non_sub	sub
NSC667558	COc1ccc(cc1)C2=C(C#N)C(=S)N([C@@H]3O[C@H](COC(=O)C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@H]3OC(=O)C)C(=C2C(=O)C)c4ccccc4	Non_sub	Non_sub	Non_sub
NSC667560	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N2C(=C(C(=O)C)C(=C(C#N)C2=S)c3occc3)C	Non_sub	Non_sub	Non_sub
NSC668354	COc1ccc(CC2=C(C3C(=O)N(N=C3c4ccccc4)c5ccccc5)C(=O)NN=C2c6ccc(C)cc6)cc1	Non_sub	sub	sub
NSC671400	S=C1N(₩C(=N/c2cccc[n+]2Cc3ccccc3)₩N(/C/1=N/c4ccccc4)c5ccccc5)c6ccccc6	Non_sub	Non_sub	Non_sub
NSC674508	Cc1cc(C)nc(NS(=O)(=O)c2ccc(Nc3c4ccccc4nc5c(cccc35)C(=O)NNCCO)cc2)n1	Non_sub	sub	sub
NSC674570	COc1ccccc1C2SCC(=O)N2c3ccc(cc3)c4ccc(cc4)N5C(=O)c6ccccc6N=C5c7ccccc7	Non_sub	Non_sub	Non_sub
NSC676593	COc1ccc(cc1)C2=C(C#N)C(=S)N(C3OC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C3OC(=O)C)C4=C2C(=O)CC(C)(C)C4	Non_sub	Non_sub	Non_sub
NSC676602	CC1=C(C#N)C(=S)N(C2OC(CO)C(O)C(O)C2O)C(=C1)C	Non_sub	Non_sub	sub
NSC676610	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N2C3=C(CCCC3)C=C(C#N)C2=S	Non_sub	Non_sub	Non_sub
NSC676615	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N2C3=C(CCCCCC3)C=C(C#N)C2=O	Non_sub	Non_sub	Non_sub
NSC676616	OCC1OC(C(O)C(O)C1O)N2C3=C(CCCCCC3)C=C(C#N)C2=S	Non_sub	Non_sub	sub
NSC676617	OCC1OC(C(O)C(O)C1O)N2C3=C(CCCC3)C=C(C#N)C2=S	Non_sub	Non_sub	sub

NSC676618	OCC1OC(C(O)C(O)C1O)N2C3=C(CCC3)C=C(C#N)C2=S	Non_sub	Non_sub	sub
NSC678047	OCC1OC(C(O)C(O)C1O)N2C(=S)C(=C3C(=C2c4cccs4)CCc5ccccc35)C#N	Non_sub	Non_sub	sub
NSC686028	CSC1=NC(=O)C(=C(N1)c2ccc(C)cc2)C#N	Non_sub	Non_sub	Non_sub
Oxprenolol	CC(C)NCC(O)COc1ccccc1OCC=C	Non_sub	Non_sub	Non_sub
Paraquat	C[n+]1ccc(cc1)c2cc[n+](C)cc2	Non_sub	Non_sub	Non_sub
Pheniramine	CN(C)CCC(c1ccccc1)c2ccccn2	Non_sub	Non_sub	Non_sub
Phosmet	COP(=S)(OC)SCN1C(=O)c2ccccc2C1=O	Non_sub	Non_sub	Non_sub
Practolol	CC(C)NCC(O)COc1ccc(NC(=O)C)cc1	Non_sub	sub	Non_sub
progesterone	CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C	Non_sub	Non_sub	Non_sub
Propranolol	CC(C)NCC(O)COc1cccc2ccccc12	Non_sub	Non_sub	Non_sub
PSC833	C₩C=C₩C[C@@H](C)C(=O)[C@@H]1N(C)C(=O)[C@H](C(C)C)N(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@H](CC(C)C)N(C)C(=O)[C@@H](C)NC(=O)[C@H](C)NC(=O)[C@H](CC(C)C)N(C)C(=O)[C@@H](NC(=O)[C@H](CC(C)C)N(C)C(=O)CN(C)C(=O)[C@@H](NC1=O)C(C)C)C(C)C	Non_sub	sub	Non_sub
Pyridostigmine	CN(C)C(=O)Oc1ccc[n+](C)c1	Non_sub	Non_sub	Non_sub
Ranitidine	CN₩C(=C/[N+](=O)[O-])₩NCCSCc1oc(CN(C)C)cc1	Non_sub	sub	Non_sub
reserpic_acid	CO[C@H]1[C@H](O)C[C@@H]2CN3CCc4c([nH]c5cc(OC)ccc45)[C@H]3C[C@@H]2[C@@H]1C(=O)O	Non_sub	sub	sub
Scopolamine	CN1[C@H]2CC(C[C@H]1[C@H]3O[C@@H]23)OC(=O)C(CO)c4ccccc4	Non_sub	sub	Non_sub
Selegiline	C[C@H](Cc1ccccc1)N(C)CC#C	Non_sub	Non_sub	Non_sub
S-Farnesyl Cysteine	OC(=O)C1=C₩C(=N₩Nc2ccc(cc2)S(=O)(=O)Nc3ccccn3)₩C=CC1=O	Non_sub	sub	Non_sub
Sulfasalazine	CNS(=O)(=O)Cc1ccc2[nH]cc(CCN(C)C)c2c1	Non_sub	Non_sub	sub
Sumatriptan	Nc1c2CCCCc2nc3ccccc13	Non_sub	sub	sub
Tacrine	CC₩C(=C(/c1ccccc1)₩c2ccc(OCCN(C)C)cc2)₩c3ccccc3	Non_sub	Non_sub	Non_sub
Tamoxifen	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O	Non_sub	sub	sub
Testosterone	Nc1nc(N)c2nc(c(N)nc2n1)c3ccccc3	Non_sub	Non_sub	Non_sub
Triamterene	ClC(Cl)(Cl)C(NC=O)N1CCN(CC1)C(NC=O)C(Cl)(Cl)Cl	Non_sub	Non_sub	Non_sub
Triforine	CC1(OC(=O)N(C1=O)c2cc(Cl)cc(Cl)c2)C=C	Non_sub	sub	sub
Vinclozolin	CC(=O)CC(C1=C(O)Oc2ccccc2C1=O)c3ccccc3	Non_sub	Non_sub	Non_sub
Warfarin	CN(C)C₩C=C(₩c1ccc(Br)cc1)/c2cccnc2	Non_sub	Non_sub	Non_sub
Zimeldine	CCCC(=O)Nc1ccc(OCC(O)CNC(C)C)c(c1)C(=O)C	Non_sub	Non_sub	sub
Acebutolol	CC(C)C1NC(=O)C(NC(=O)C2=C(N)C(=O)C(=C	sub	sub	sub

	3Oc4c(C)ccc(C(=O)NC5C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C6CCCN6C(=O)C(NC5=O)C(C)C)c4N=C23)C)C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C7CCCN7C1=O			
Actinomycin	CC(C)C1NC(=O)C(NC(=O)C2=C(N)C(=O)C(=C3Oc4c(C)ccc(C(=O)NC5C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C6CCCN6C(=O)C(NC5=O)C(C)C)c4N=C23)C)C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C7CCCN7C1=O	sub	sub	sub
actinomycin_d	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5C[C@H](N)[C@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)CO	sub	sub	sub
adriamycin	C[C@]12CCC(=O)C=C1CC[C@H]3[C@@H]4CC[C@H](C(=O)CO)[C@]4(C[C@H](O)[C@H]23)C=O	sub	sub	sub
Aldosterone	CCCCc1oc2ccccc2c1C(=O)c3cc(I)c(OCCN(CC)CC)c(I)c3	sub	sub	sub
Amiodarone	CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)c3ccc(O)cc3)C(=O)N2[C@H]1C(=O)O	sub	sub	sub
amoxicillin	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)O[C@H]2CCOC2)S(=O)(=O)c3ccc(N)cc3	sub	Non_sub	Non_sub
Amprenavir	COc1ccc(CCN2CCC(CC2)Nc3nc4ccccc4n3Cc5ccc(F)cc5)cc1	sub	sub	sub
Astemizole	CCOC(=O)C1=C(C)NC(=C(C1c2ccccc2C(F)(F)F)C(=O)OCCNC(=O)c3ccc(cc3)N=[N+]=[N-])C	sub	sub	sub
Azidopine	CC(C)COC[C@H](CN(Cc1ccccc1)c2ccccc2)N3CCCC3	sub	sub	sub
Bepridil	C1CN=C(N₩N=C₩c2c3ccccc3c(₩C=N₩NC4=NCCN4)c5ccccc25)N1	sub	sub	sub
Bisantrene	CC(C)(C)NCC(O)COc1ccccc1C#N	sub	sub	sub
bunitrolol	COC1=CC(=O)c2c(O)c(OC)c(CC(C)OC(=O)Oc3ccc(O)cc3)c4c2c1c5C(=CC(=O)c6c(O)c(OC)c(CC(C)OC(=O)c7ccccc7)c4c56)OC	sub	Non_sub	Non_sub
Calphostin C	CCC1=C[C@H]2CN3CCc4c([nH]c5ccccc45)[C@@](C2)([C@@H]13)C(=O)OC	sub	sub	sub
catharanthine	Cc1nnc(SCC2=C(N3[C@H](SC2)[C@H](NC(=O)Cn4cnnn4)C3=O)C(=O)O)s1	sub	sub	sub
Cefazolin	CCN1CCN(C(=O)NC(C(=O)N[C@H]2[C@H]3SCC(=C(N3C2=O)C(=O)O)CSc4nnnn4C)c5ccc(O)cc5)C(=O)C1=O	sub	sub	Non_sub
Cefoperazone	CO[C@]1(NC(=O)C2SC(=C(C(=O)N)C(=O)O)S2)C3SCC(=C(N3C1=O)C(=O)O)CSc4nnnn4C	sub	sub	sub
Cefotetan	CCN(CC)C(=O)Nc1ccc(OCC(O)CNC(C)(C)C)c(c1)C(=O)C	sub	sub	sub
Celiprolol	COc1ccc2C[C@H]3N(C)CCc4cc(OC)c(Oc5c6OCOc6cc7CCN(C)[C@@H](Cc8ccc(Oc1c2)cc8)c57)cc34	sub	sub	sub
Cepharanthine	CCN(CC)CCCC(C)Nc1ccnc2cc(Cl)ccc12	sub	sub	sub

Chloroquine	C₩N=C(₩NCCSCc1nc[nH]c1C)/NC#N	sub	sub	sub
Cimetidine	OC(C1CC2CCN1CC2C=C)c3ccnc4ccccc34	sub	sub	sub
Cinchonidine	OC(=O)C1=CN(C2CC2)c3cc(N4CCNCC4)c(F)cc3C1=O	sub	sub	sub
ciprofloxacin	OCCN1CCN(CC₩C=C/2₩c3ccccc3Sc4ccc(cc24)C(F)(F)F)CC1	sub	sub	Non_sub
cis-flupenthixol	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]3O[C@H](C)C[C@@H]([C@H]3O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)OC	sub	sub	sub
clarithromycin	Clc1ccccc1C(c2ccccc2)(c3ccccc3)n4ccnc4	sub	sub	sub
Clotrimazole	COC1=CC=C2C(=CC1=O)[C@H](CCc3cc(OC)c(OC)c(OC)c23)NC(=O)C	sub	Non_sub	Non_sub
Colchicine	C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2C(=O)CO	sub	sub	Non_sub
Corticosterone	C[C@]12CCC(=O)C=C1CC[C@H]3[C@@H]4CC[C@](O)(C(=O)CO)[C@@]4(C)C[C@H](O)[C@H]23	sub	sub	sub
cortisol	COc1ccc(CCNc2nc(N3CCc4cc(OC)c(OC)cc4C3)c5cc(OC)c(OC)cc5n2)cc1OC	sub	sub	sub
CP100356	CCC1NC(=O)C(C(O)C(C)C₩C=C₩C)N(C)C(=O)C(C(C)C)N(C)C(=O)C(CC(C)C)N(C)C(=O)C(CC(C)C)N(C)C(=O)C(C)NC(=O)C(C)NC(=O)C(CC(C)C)N(C)C(=O)C(NC(=O)C(CC(C)C)N(C)C(=O)CN(C)C1=O)C(C)C	sub	sub	sub
Cyclosporin A	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5C[C@H](N)[C@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)C	sub	sub	sub
Daunomycin	NC(=N)N1CCc2ccccc2C1	sub	sub	sub
debrisoquine	C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO	sub	Non_sub	Non_sub
Dexamethasone	CCCN1C(=C([C@H](C(=C1C)C(=O)ON2CCC(CC2)(c3ccccc3)c4ccccc4)c5cccc(c5)[N+](=O)[O-])C(=O)OC)C	sub	sub	sub
Dexniguldipine	CCCCOc1cc(C(=O)NCCN(CC)CC)c2ccccc2n1	sub	Non_sub	sub
Dibucaine	C[C@]12CC[C@H](O)C[C@H]1CC[C@@H]3[C@@H]2CC[C@]4(C)[C@H](CC[C@]34O)C5=CC(=O)OC5	sub	sub	sub
Digitoxigenin	C[C@H]1O[C@H](C[C@H](O)[C@@H]1O)O[C@H]2[C@@H](O)C[C@H](O[C@H]3[C@@H](O)C[C@H](O[C@H]4CC[C@@]5(C)[C@H](CC[C@@H]6[C@@H]5CC[C@]7(C)[C@H](CC[C@]67O)C8=CC(=O)OC8)C4)O[C@@H]3C)O[C@@H]2C	sub	sub	sub

Digitoxin	C[C@]12CC[C@H](O)C[C@H]1CC[C@@H]3[C@@H]2C[C@@H](O)[C@]4(C)[C@H](CC[C@]34O)C5=CC(=O)OC5	sub	sub	sub
Digoxigenin	C[C@H]1O[C@H](C[C@H](O)[C@@H]1O)O[C@H]2[C@@H](O)C[C@H](O[C@H]3[C@@H](O)C[C@H](O[C@H]4CC[C@@]5(C)[C@H](CC[C@@H]6[C@@H]5C[C@@H](O)[C@]7(C)C(CC[C@]67O)C8=CC(=O)OC8)C4)O[C@@H]3C)O[C@@H]2C	sub	sub	sub
Digoxin	OCCN(CCO)c1nc(N2CCCCC2)c3nc(nc(N4CCCCC4)c3n1)N(CCO)CCO	sub	sub	sub
Dipyridamole	CC(=O)O[C@@]12CO[C@@H]1C[C@H](O)[C@]3(C)[C@@H]2[C@H](OC(=O)c4ccccc4)[C@]5(O)C[C@H](OC(=O)[C@H](O)[C@@H](NC(=O)OC(C)(C)C)c6ccccc6)C(=C([C@@H](O)C3=O)C5(C)C)C	sub	sub	sub
Docetaxel	Clc1ccc2N(C3CCN(CCCN4C(=O)Nc5ccccc45)CC3)C(=O)Nc2c1	sub	sub	sub
Domperidone	FC(F)(F)[C@]1(OC(=O)Nc2ccc(Cl)cc12)C#CC3CC3	sub	sub	sub
efavirenz	CN1CCC[C@@H]1Cc2c[nH]c3ccc(CCS(=O)(=O)c4ccccc4)cc23	sub	sub	Non_sub
eletriptan	CC[C@H]1CN2CCc3cc(OC)c(OC)cc3[C@@H]2C[C@@H]1C[C@H]4NCCc5cc(OC)c(OC)cc45	sub	sub	sub
Emetine	ClC1=C(Cl)C2(Cl)C3COS(=O)OCC3C1(Cl)C2(Cl)Cl	sub	sub	sub
Endosulfan	CCN1C=C(C(=O)O)C(=O)c2cc(F)c(nc12)N3CCNCC3	sub	Non_sub	Non_sub
enoxacin	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5C[C@H](N)[C@@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)CO	sub	Non_sub	Non_sub
epirubicin	C[C@H]1CCC[C@H]2O[C@H]2C[C@H](OC(=O)C[C@H](O)C(C)(C)C(=O)[C@H](C)[C@H]1O)₩C(=C₩c3csc(C)n3)₩C	sub	sub	sub
epothilone_a	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]3O[C@H](C)C[C@@H]([C@H]3O)N(C)C)[C@](C)(O)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O	sub	sub	sub
Erythromycin	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O	sub	sub	sub
estradiol	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](O)[C@@H]2O	sub	sub	sub
Estriol	COc1cc(cc(OC)c1O)[C@H]2[C@@H]3[C@H](COC3=O)[C@H](O[C@@H]4O[C@@H]5CO[C@@H](C)O[C@H]5[C@H](O)[C@H]4O)c6cc7OCOc7cc26	sub	sub	sub
Etoposide	CC(C)(C(=O)O)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c3ccccc3)c4ccccc4	sub	sub	sub

fexofenadine	CN1C(=O)CN=C(c2ccccc2F)c3cc(ccc13)[N+](=O)[O-]	sub	sub	sub
flunitrazepam	OCCN1CCN(CCCN2c3ccccc3Sc4ccc(cc24)C(F)(F)F)CC1	sub	Non_sub	Non_sub
Fluphenazine	COc1ccc(CCN(C)CCCC(C#N)(C(C)C)c2cc(OC)c(OC)c(OC)c2)cc1OC	sub	sub	sub
Gallopamil	OC1(CCN(CCCC(=O)c2ccc(F)cc2)CC1)c3ccc(Cl)cc3	sub	sub	sub
haloperidol	C[C@]12CCC(=O)C=C1CC[C@H]3[C@@H]4CC[C@](O)(C(=O)CO)[C@@]4(C)C[C@H](O)[C@H]23	sub	sub	sub
Hydrocortisone	COc1cccc2C(=O)c3c(O)c4C[C@](O)(C[C@H](O[C@H]5CC(O)[C@H](O)[C@H](C)O5)c4c(O)c3C(=O)c12)C(=O)CO	sub	sub	sub
Hydroxyrubicin	C[C@@H]1O[C@H](C[C@H](N)[C@@H]1O)O[C@H]2C[C@@](O)(Cc3c(O)c4C(=O)c5ccccc5C(=O)c4c(O)c23)C(=O)C	sub	sub	sub
Idarubicin	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	sub	sub	sub
Indinavir	CCc1c2CN3C(=O)C4=C(C=C3c2nc5ccc(OC(=O)N6CCC(CC6)N7CCCCC7)cc15)[C@@](O)(CC)C(=O)OC4	sub	sub	sub
irinotecan	C₩C=C₩c1ccc2OCOc2c1	sub	sub	sub
Isosafrole	CCC(C)C1O[C@]2(CCC1C)C[C@@H]3CC(C₩C=C(/C)₩C(O[C@H]4C[C@H](OC)C(O[C@H]5C[C@H](OC)C(O)[C@H](C)O5)[C@H](C)O4)C(C)₩C=C₩C=C₩6/COC7[C@H](O)C(=C[C@@H](C(=O)O3)C67O)C)O2	sub	Non_sub	Non_sub
Ivermectin	CCN(CC)C(=O)c1c2C[C@H](C)CCc2sc1NC(=O)c3cccs3	sub	sub	sub
k02	N[C@@H](Cc1ccc(O)c(O)c1)C(=O)O	sub	sub	sub
L_dopa	CC(C)C[C@H](NC(CCCN=C(N)N)C=O)C(=O)NC(=O)[C@H](CC(C)C)NC(=O)C	sub	Non_sub	Non_sub
Leupeptin	C[C@H]1COc2c(N3CCN(C)CC3)c(F)cc4C(=O)C(=CN1c24)C(=O)O	sub	sub	sub
levofloxacin	COc1ccc2Sc3ccccc3N(CC(C)CN(C)C)c2c1	sub	sub	Non_sub
Levomeprazine	CN(C)C(=O)C(CCN1CCC(O)(CC1)c2ccc(Cl)cc2)(c3ccccc3)c4ccccc4	sub	sub	sub
Loperamide	CCOC(=O)N1CCC(=C2c3ccc(Cl)cc3CCc4cccnc24)CC1	sub	sub	sub
loratidine	CCCCc1nc(Cl)c(CO)n1Cc2ccc(cc2)c3ccccc3c4nn[nH]n4	sub	Non_sub	Non_sub
losartan	CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@@H]12	sub	sub	sub
Lovastatin	O[C@@H](COc1cccc2ncccc12)CN3CCN(CC3)C4c5ccccc5[C@H]6[C@@H](c7ccccc47)C6(F)F	sub	sub	sub

LY335979	C(C1CN2CCC1CC2)N3c4ccccc4Sc5ccccc35	sub	sub	sub
Mequitazine	CCC(=O)C(CC(C)N(C)C)(c1ccccc1)c2ccccc2	sub	sub	sub
Methadone	C[C@H]1C[C@H]2[C@@H]3CC[C@](O)(C(=O)CO)[C@@]3(C)C[C@H](O)[C@@H]2[C@@]4(C)C=CC(=O)C=C14	sub	Non_sub	Non_sub
Methylprednisolone	CCOC(=O)Oc1c(OC)cc(cc1OC)C(=O)O[C@@H]2C[C@@H]3CN4CCc5c([nH]c6cc(OC)ccc56)[C@H]4C[C@@H]3[C@@H]([C@H]2OC)C(=O)OC	sub	sub	sub
Methylreserpate	CO[C@@H]([C@@H]1Cc2cc3cc(O[C@H]4C[C@@H](O[C@H]5C[C@@H](O)[C@H](O)[C@@H](C)O5)[C@H](O)[C@@H](C)O4)c(C)c(O)c3c(O)c2C(=O)[C@H]1O[C@H]6C[C@@H](O[C@H]7C[C@@H](O[C@H]8C[C@](C)(O)[C@H](O)[C@@H](C)O8)[C@@H](O)[C@@H](C)O7)[C@H](O)[C@@H](C)O6)C(=O)[C@@H](O)[C@@H](C)O	sub	sub	sub
mithramycin	CO[C@]12[C@H]3N[C@H]3CN1C4=C([C@H]2COC(=O)N)C(=O)C(=C(C)C4=O)N	sub	sub	sub
mitomycin	OCCNCCNc1ccc(NCCNCCO)c2C(=O)c3c(O)ccc(O)c3C(=O)c12	sub	Non_sub	sub
Mitoxantrone	CC[C@]1(CC[C@@H](O1)[C@@]2(C)CC[C@]3(C[C@H](O)[C@@H](C)[C@H](O3)[C@H](C)[C@H](OC)[C@@H](C)C(=O)O)O2)[C@H]4O[C@@H](C[C@H]4C)[C@H]5O[C@@](O)(CO)[C@H](C)C[C@@H]5C	sub	sub	sub
Monensin	CN1CC[C@]23[C@H]4Oc5c(O)ccc(C[C@@H]1[C@@H]2C=C[C@@H]4O)c35	sub	sub	sub
Morphine	CN1CC[C@]23[C@H]4Oc5c(O)ccc(C[C@@H]1[C@@H]2C=C[C@@H]4O[C@@H]6O[C@@H]([C@@H](O)[C@H](O)[C@H]6O)C(=O)O)c35	sub	sub	sub
morphine-6-glucuronide	C[C@H]1C[C@H]2[C@@H]3CC[C@](O)(C(=O)CO)[C@@]3(C)C[C@H](O)[C@@H]2[C@@]4(C)C=CC(=O)C=C14	sub	Non_sub	sub
m-prednisolone	CCC1=CC2CN(C1)Cc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](OC(=O)C)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)OC	sub	sub	sub
navelbine	CCC1=NN(CCCN2CCN(CC2)c3cccc(Cl)c3)C(=O)N1CCOc4ccccc4	sub	sub	sub
nefazodone	Cc1c(O)cccc1C(=O)N[C@@H](CSc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	sub	sub	sub
Nelfinavir	Cc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12	sub	sub	sub
nevirapine	COCCOC(=O)C1=C(C)NC(=C(C1c2cccc(c2)[N+](=O)[O-])C(=O)OC(C)C)C	sub	Non_sub	Non_sub
Nimodipine	CNCCC=C1c2ccccc2CCc3ccccc13	sub	sub	sub
nortriptyline	CC1COC2(CC1OC(=O)₩C=C₩c3ccccc3)OC4C	sub	Non_sub	Non_sub

	C(CCC4C25CO5)C(=O)OC6OC(C)C(O)C(OC(=O)C)C6OC7OC(C)C(O)C(OC(=O)C)C7O			
NSC328426	CC(C)C1NC(=O)C(NC(=O)c2ccc(C)c3Oc4c(C)c5OC(=O)C(=Nc5c(C(=O)NC6C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C7CCCN7C(=O)C(NC6=O)C(C)C)c4Nc23)c8ccccc8)C(C)OC(=O)C(C(C)C)N(C)C(=O)CN(C)C(=O)C9CCCN9C1=O	sub	sub	sub
NSC339281	CCN(CC)CC[n+]1ccc2c(C)c3[nH]c4ccccc4c3c(C)c2c1	sub	sub	sub
NSC359449	C₩C=C₩1/NC(=O)[C@H]2CSSCC₩C=C₩[C@H](CC(=O)N[C@H](C(C)C)C(=O)N2)OC(=O)[C@@H](NC1=O)C(C)C	sub	sub	sub
NSC630176	CC[n+]1c(₩C=C₩c2ccc(cc2)N(CCCl)CCCl)ccc3cc(NC(=O)₩C=C₩c4ccccc4)ccc13	sub	sub	sub
NSC640085	CN1CCC=CC1	sub	sub	sub
NSC66490	Cc1nccn1CC2CCc3c(C2=O)c4ccccc4n3C	sub	Non_sub	Non_sub
Ondansetron	CC(=O)O[C@H]1C(=O)[C@]2(C)[C@@H](O)C[C@H]3OC[C@@]3(OC(=O)C)[C@H]2[C@H](OC(=O)c4ccccc4)[C@]5(O)C[C@H](OC(=O)[C@H](O)[C@@H](NC(=O)c6ccccc6)c7ccccc7)C(=C1C5(C)C)C	sub	Non_sub	Non_sub
Paclitaxel	CC(C)NCC(O)COc1ccc(CCNC(=O)NC(C)C)cc1	sub	sub	sub
Pafenolol	Nc1ccc(cc1)C(=C2C=CC(=N)C=C2)c3ccc(N)cc3	sub	sub	sub
pararosaniline	OCCN1CCN(CCCN2c3ccccc3Sc4ccc(Cl)cc24)CC1	sub	sub	sub
Perphenazine	CCC1(C(=O)NC(=O)NC1=O)c2ccccc2	sub	sub	sub
Phenobarbital	N1c2ccccc2Oc3ccccc13	sub	Non_sub	Non_sub
Phenoxazine	O=C1NC(=O)C(N1)(c2ccccc2)c3ccccc3	sub	Non_sub	Non_sub
Phenytoin	Fc1ccc(cc1)C(CCCN2CCC(CC2)N3C(=O)Nc4ccccc34)c5ccc(F)cc5	sub	Non_sub	Non_sub
Pimozide	COc1cc2nc(nc(N)c2cc1OC)N3CCN(CC3)C(=O)c4occc4	sub	sub	sub
Prazosin	CN(C)CCCN1c2ccccc2Sc3ccccc13	sub	Non_sub	Non_sub
promazine	CNCCCC1c2ccccc2C=Cc3ccccc13	sub	sub	sub
Protriptyline	COc1ccc(C[C@H](N)C(=O)NC2C(CO)OC(C2O)n3cnc4c(ncnc34)N(C)C)cc1	sub	Non_sub	Non_sub
Puromycin	COc1ccc2nccc([C@H](O)[C@H]3C[C@@H]4CCN3C[C@@H]4C=C)c2c1	sub	Non_sub	sub
Quinidine	COc1ccc2nccc([C@@H](O)[C@@H]3CC4CCN3C[C@@H]4C=C)c2c1	sub	sub	sub
Quinine	CO[C@@H]1C[C@H](C[C@@H](C)[C@@H]2CC(=O)[C@H](C)₩C=C(/C)₩[C@@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)₩C=C/C=C/C=C(₩C)/[C@H](C[C@@H]3CC[C@@H](C)[C@@](O)(O3)C(=O)C(=O)N4CCCC[C@H]4C(=O)O2)OC)CC[C@H]1O	sub	sub	sub

Rapamycin	CO[C@H]1[C@@H](C[C@@H]2CN3CCc4c([nH]c5cc(OC)ccc45)[C@H]3C[C@@H]2[C@@H]1C(=O)OC)OC(=O)c6cc(OC)c(OC)c(OC)c6	sub	sub	sub
Reserpine	COC(=O)c1ccccc1C2=C3C=CC(=[NH2+])C=C3Oc4cc(N)ccc24	sub	sub	sub
Rhodamine 123	CO[C@H]1₩C=C₩O[C@@]2(C)Oc3c(C)c(O)c4C(=C(NC(=O)₩C(=C/C=C/[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(=O)C)[C@@H]1C)₩C)₩C(=C/NN5CCN(C)CC5)₩C(=O)c4c3C2=O)O	sub	sub	sub
Rifampicin	CC1=C(CCN2CCC(CC2)c3noc4cc(F)ccc34)C(=O)N5CCCCC5=N1	sub	sub	sub
Risperidone	CC(C)[C@H](NC(=O)N(C)Cc1csc(n1)C(C)C)C(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3cncs3)Cc4ccccc4	sub	sub	sub
Ritonavir	Fc1ccc(cc1)C(CNC2CCN(CC2)c3nc(NCC=C)nc(NCC=C)n3)c4ccc(F)cc4	sub	sub	sub
S9788	CCCCCCCCCCCCCCC[C@@H](O)[C@@H](N)CO	sub	sub	sub
Safingol	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4	sub	sub	sub
Saquinavir	CC(=CCC₩C(=C₩CC₩C(=C₩CSC[C@H](N)C(=O)O)₩C)₩C)C	sub	sub	sub
sparfloxacin	C[C@@H]1CN(C[C@H](C)N1)c2c(F)c(N)c3C(=O)C(=CN(C4CC4)c3c2F)C(=O)O	sub	sub	sub
Spiperone	Fc1ccc(cc1)C(=O)CCCN2CCC3(CC2)N(CNC3=O)c4ccccc4	sub	sub	sub
Staurosporine	CN[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n3c4ccccc4c5c6CNC(=O)c6c7c8ccccc8n2c7c35	sub	sub	sub
Tacrolimus	CO[C@@H]1CC(CC[C@H]1O)₩C=C(/C)₩[C@H]2OC(=O)[C@@H]3CCCCN3C(=O)C(=O)[C@]4(O)O[C@H]([C@H](C[C@@H](C)C₩C(=C₩[C@@H](CC=C)C(=O)C[C@H](O)[C@H]2C)₩C)OC)[C@H](C[C@H]4C)OC	sub	sub	sub
talinolol	CC(C)(C)NCC(O)COc1ccc(NC(=O)NC2CCCCC2)cc1	sub	sub	sub
taxol	CC(=O)O[C@H]1C(=O)[C@]2(C)[C@@H](O)C[C@H]3OC[C@@]3(OC(=O)C)[C@H]2[C@H](OC(=O)c4ccccc4)[C@]5(O)C[C@H](OC(=O)[C@H](O)[C@@H](NC(=O)c6ccccc6)c7ccccc7)C(=C1C5(C)C)C	sub	sub	sub
Teniposide	COc1cc(cc(OC)c1O)[C@H]2[C@@H]3[C@H](COC3=O)[C@H](O[C@@H]4O[C@@H]5CO[C@@H](O[C@H]5[C@H](O)[C@H]4O)c6cccs6)c7cc8OCOc8cc27	sub	sub	sub
Terfenadine	CC(C)(C)c1ccc(cc1)C(O)CCCN2CCC(CC2)C(O)(c	sub	sub	sub

	3ccccc3)c4ccccc4			
tetraphenylphosphonium	c1ccc(cc1)[P+](c2ccccc2)(c3ccccc3)c4ccccc4	sub	Non_sub	Non_sub
Thioridazine	CSc1ccc2Sc3ccccc3N(CCC4CCCCN4C)c2c1	sub	sub	sub
Topotecan	CC[C@@]1(O)C(=O)OCC2=C1C=C3N(Cc4cc5c(CN(C)C)c(O)ccc5nc34)C2=O	sub	sub	sub
Toremifene	CN(C)CCOc1ccc(cc1)₩C(=C(₩CCCl)/c2ccccc2)₩c3ccccc3	sub	sub	sub
trazodone	Clc1cccc(c1)N2CCN(CCCN3N=C4C=CC=CN4C3=O)CC2	sub	sub	sub
Trifluoperazine	CN1CCN(CCCN2c3ccccc3Sc4ccc(cc24)C(F)(F)F)CC1	sub	sub	sub
Triflupromazine	CN(C)CCCN1c2ccccc2Sc3ccc(cc13)C(F)(F)F	sub	sub	sub
Trimethoprim	COc1cc(Cc2cnc(N)nc2N)cc(OC)c1OC	sub	Non_sub	Non_sub
Valinomycin	CC(C)C1NC(=O)C(C)OC(=O)C(NC(=O)C(OC(=O)C(NC(=O)C(C)OC(=O)C(NC(=O)C(OC(=O)C(NC(=O)C(C)OC(=O)C(NC(=O)C(OC1=O)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C)C(C)C	sub	sub	sub
Vinblastine	CC[C@]1(O)C[C@@H]2CN(CCc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](OC(=O)C)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)OC)C1	sub	sub	sub
Vincristine	CC[C@]1(O)C[C@H]2CN(CCc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C=O)[C@H]7[C@](O)([C@H](OC(=O)C)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)OC)C1	sub	sub	sub
vindesine	CC[C@]1(O)C[C@H]2CN(CCc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](O)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)N)C1	sub	sub	sub
Vindoline	CCC12C=CCN3CC[C@@]4([C@H]13)[C@@H](N(C)c5cc(OC)ccc45)[C@](O)([C@@H]2OC(=O)C)C(=O)OC	sub	sub	sub
vinorelbine	CCC1=CC2CN(C1)Cc3c([nH]c4ccccc34)[C@@](C2)(C(=O)OC)c5cc6c(cc5OC)N(C)[C@H]7[C@](O)([C@H](OC(=O)C)[C@]8(CC)C=CCN9CC[C@]67[C@H]89)C(=O)OC	sub	sub	sub